Computational Chemistry: An Emerging Technology for Solving Problems in Atmospheric Chemistry

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Over the past three decades, atmospheric chemistry has served as an important component in developing strategies for reducing ambient concentrations of air pollutants. Laboratory studies are carried out to investigate the key chemical reactions that determine the fates and lifetimes of air pollutants, with the resulting data used to develop air quality models for predicting their ambient concentrations. Carefully planned field studies are carried out to evaluate the air quality models. If the models are found to be reliable, they are used by EPA and the states for various regulatory activities to evaluate control strategies for meeting national air quality standards. To date, these models have been employed to evaluate strategies for ozone, air toxic compounds and particulate matter. While this methodology has led to significant improvements in air quality, the large amount of input data needed for the models and the cost and time required for laboratory studies has limited the number of modeling studies completed. However, over the past decade, rapid advances in computational chemistry have led to the development of software tools for predicting chemical properties such as activity coefficients, solubilities, vapor pressures and atmospheric lifetimes and fates of atmospherically relevant compounds. These tools have the potential for providing the agency with the chemical input data required for air quality models in a rapid and cost-effective manner.

A series of screening studies have been carried out to evaluate the reliability of computational chemistry-based predictions of thermodynamic and kinetic data of atmospherically relevant compounds. Studies conducted to date include the use of computational chemistry to predict (1) the atmospheric lifetimes of substitutes of ozone-depleting chlorofluorocarbons, (2) the atmospheric fate of toluene, a key component of automobile exhaust, (3) the atmospheric lifetime of mercury, and (4) the vapor pressures and activity coefficients of organic compounds in $PM_{2.5}$. While additional studies are needed to fully evaluate this new tool, the results suggest that computational chemistry-based methods could play an important role in assessing control strategies for reducing ambient concentrations of air pollutants. Furthermore, even at this stage of development, there has been an integration of computational chemistry into research being carried out by NERL scientists as shown by the computational chemistry-based vapor pressures and activity coefficients of organic compounds serving as input data for the PM chemistry model to be used by OAQPS and in state implementation plans.

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